CLOSED ORBITS AND RECURRENCES IN ATOMIC SPECTRA: PATTERNS OF TRAJECTORIES IN INTEGRABLE SYSTEMS

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Abstract

A simple harmonic-barrier model shows the same patterns of closed orbits that have been found in calculations on atomic systems.

We start with an atom placed in electric and/or magnetic fields. Laser light (either short-pulse or continuous-wave) excites an electron either to high-energy bound states or to free states. The electron travels away from the atom and is acted upon by the applied fields. Depending on its energy and its initial direction of motion, the electron may some time later return to the atom. Such a return we call a recurrence, and these recurrences are plainly visible in absorption spectra. With sufficiently short pulses, recurrences are visible in real time;\(^1\) with cw lasers, recurrences manifest themselves as interference effects in absorption spectra.\(^2\)

A general theory of the effects of recurrences on atomic spectra has been developed\(^3\) ("Closed-Orbit Theory" and "Recurrence Spectroscopy"). The theory makes use of semiclassical approximations—from numerically generated classical trajectories of the active electron, the theory constructs those relevant parts of the wave function that are needed to calculate the absorption spectrum. Closed classical orbits are therefore the input to the theory, and the output is a measurable quantity that we call the "recurrence strength" of each orbit.

In our computations of classical orbits of the electron, certain patterns show up repeatedly. Figure 1 shows a family of closed orbits of an electron moving in a combined Coulomb field and static electric field (Stark system).\(^4\) Sequences of orbits having similar shapes occur for an electron in Coulomb and magnetic fields,\(^5,6\) constant electric and magnetic fields,\(^6\) and Coulomb and parallel field.\(^7\)

In this paper we present a simple, exactly solvable model that helps us understand these patterns. We then show the relationship between this model and the Stark system.
1. **Harmonic-Barrier Model**

We consider a Hamiltonian representing a quadratic well in the $x$ direction and a quadratic barrier in the $y$ direction,

$$
H = \frac{1}{2m} (p_x^2 + p_y^2) + \frac{1}{2} (k_x x^2 - k_y y^2) = E .
$$  \hspace{1cm} (1)

Let us consider a family of orbits subject to the following initial conditions. All orbits have the same total energy, and all emerge from a single point on the negative $y$ axis ($x = 0, y = -y_0$), moving outward in any direction in the $xy$ plane. Which of these orbits return to the initial point? We wish to (a) list the closed orbits (COs), (b) evaluate the classical action on each CO, and (c) evaluate the classical amplitude on each CO. We will show that there is an orderly sequence of closed orbits that approach an unstable periodic orbit (PO) sitting on top of the barrier (Fig. 2), that actions of adjacent members

Fig. 2. Four of the closed orbits of the harmonic barrier model.
of the sequence differ by the action of the unstable PO (Eq. 10), and that the classical amplitudes of adjacent members of the sequence differ by a Liapunov factor associated with that orbit (Eq. 14).

1.1 Closed Orbits

The energy in each mode is conserved:

$$E_x = \frac{p_x^2}{2m} + \frac{1}{2} k_x x^2 \quad E_y = \frac{p_y^2}{2m} - \frac{1}{2} k_y y^2 ,$$

with $$E = E_x + E_y$$. The motion in the $$(p_x, x)$$ plane is stable, while the motion in the $$(p_y, y)$$ plane is unstable. There exists one unstable periodic orbit (the "ridge orbit") that sits on top of the barrier with $$y = 0$$, $$p_y = 0$$, $$E_y = 0$$, $$E_x = E$$. Its action is $$S_{un} = 2\pi E/\omega_x$$ with $$\omega_x = \sqrt{k_x/m} = 2\pi/T_{un}$$. Its neighbors diverge from it exponentially, as $$\exp(\pm \omega_x t)$$, with $$\omega_x = \sqrt{k_x/m}$$ being the Liapunov exponent. We define the Liapunov factor for this orbit as

$$\lambda_{un} = \omega_y T_{un} = 2\pi \omega_y / \omega_x .$$

Orbits start at $$t=0$$ from the negative $$y$$ axis and with $$x_0 = 0$$, so the closed orbits must satisfy the conditions $$0 < p_{yo} < \sqrt{mk_y} |y_o|$$ and $$E_y < 0$$. The orbital equations are

$$x(t) = A \sin(\omega_x t) \quad y(t) = B \cosh(\omega_y t + \alpha) ,$$

where $$A = \sqrt{2E_x/k_x}$$ and $$B = \sqrt{-2E_y/k_y}$$. We will show that each closed orbit can be labeled by a single positive integer, and, for consistency with the following section, we will give each orbit the "name" $$l/l$$, with $$l$$ an integer. A closed orbit satisfies $$y_l = y_o$$, $$x_l = 0$$, so the closure time of the orbit is an integer number of half-cycles of $$x$$ motion, $$T_{1/l} = l\pi/\omega_x$$. Hence,

$$B_{1/l} = \frac{y_o}{\cosh(l\pi \omega_y / 2 \omega_x)} , \quad A_{1/l} = \sqrt{\frac{2(E + k_x B_{1/l}^2/2)}{k_x}} , \quad \alpha = -l\pi \omega_y / 2 \omega_x .$$

Also, $$y(t)$$ reaches a maximum at half the closure time, and at that moment,

$$\dot{x} = \omega_x A \cos(l\pi/2) .$$

If $$l$$ is odd, both $$\dot{x}$$ and $$\dot{y}$$ vanish simultaneously, and the orbit has an endpoint, while if $$l$$ is even, $$\dot{x}$$ is finite and $$x = 0$$ when $$y$$ is a maximum. Therefore the closed orbits form an alternating sequence of "balloons" and "snakes" (Fig. 2). The maximum value of $$y$$ is the minimum distance of the closed orbit from the ridge orbit, and it is equal to $$B_{1/l}$$, which for large $$l$$ is approximately
\[ B_{v_{II}} = y_0 \exp(-l\pi \omega / 2\omega_y) \quad . \] (6)

1.2. Classical Action

The action associated with \( x \) motion on each full cycle is very simple—it equals the area enclosed by the ellipse in the \((P_x, x)\) plane.

The action of \( y \) motion from start to closure is

\[
S_x = \oint P_x dx = \oint [2m/(E - k x^2)]^{1/2} dx = \frac{2\pi E_x}{\omega_x} \quad .
\] (7)

\[
S_y = 2\sqrt{mk_y} \int_{b_y}^{\gamma_y} \sqrt{y^2 + 2Ex_y/k_y} \ dy \quad .
\] (8)

so the total action is the combination of the \( y \)-action plus the \( x \)-action on \( l \) half-cycles,

\[
S_{v_{II}} = l\pi \frac{E_x}{\omega_x} + 2\sqrt{mk_y} \int_{b_y}^{\gamma_y} \sqrt{y^2 - B_{v_{II}}^2} \ dy
\]

\[
= l\pi \frac{E_x}{\omega_x} + \sqrt{mk_y} \frac{y_0^2}{2} + O(e^{-l\beta_1/\omega_y}) \quad \text{for large } l \quad .
\] (9)

Hence as \( l \) increases, the energy of \( y \) motion \( E_y \) approaches zero from below, and the action difference of successive orbits is equal to

\[
S_{v_{II,-1}} - S_{v_{II}} \approx \pi E / \omega_y = S_{\infty} / 2 \quad ,
\] (10)

which equals the action of a half-cycle of the unstable PO that lies on the ridge.

1.3. Classical Amplitude

The amplitude of returning waves associated with the family of orbits surrounding any closed orbit (the "classical amplitude") is related to the element of the Jacobian matrix \( J_{12} \) by \( A \propto |J_{12}|^{-1/2} \).

\[
J_{12} = \left[ \begin{array}{c} \frac{\partial y}{\partial p_{x_s}} \\ \cdots \end{array} \right]_{x_s} \quad .
\] (11)
Since

\[ y = \sqrt{\frac{-2E_y}{k_y}} \cosh \left( \omega_y t - \frac{l\pi \omega_y}{2\omega_x} \right), \quad (12) \]

so

\[ J_{12} = -\frac{p_{y_0}}{mk_y y_0} \cosh^2 \frac{l\pi \omega_y}{2\omega_x} \]
\[ = -\frac{p_{y_0}}{4mk_y y_0} \exp \left( l\pi \omega_y / \omega_x \right) \text{ (for large } l \text{).} \quad (13) \]

When \( l \) is large, the initial momentum of closed orbits becomes approximately independent of \( l \). Therefore, the amplitude ratio of two successive orbits is

\[ \frac{A_{1/(l+1)}}{A_{1/l}} = \exp \left( -\pi \omega_y / 2\omega_x \right) = \exp \left( -\omega_y T_{\infty} / 4 \right) \]
\[ = \exp \left( -\lambda_{\infty} / 4 \right). \quad (14) \]

Next we shall see that similar results can be derived in a real physical system.

2. Atoms in an Electric Field

The Stark Hamiltonian is conveniently written in scaled semiparabolic coordinates as

\[ h = \frac{1}{2} \left( p_u^2 + p_v^2 \right) + V(u, v) = 2, \]
\[ V(u, v) = \frac{1}{2} (u^4 - v^4) - \epsilon (u^2 + v^2), \]
\[ \epsilon = E/F^{1/2}. \quad (15) \]

(See Fig. 3.) This Hamiltonian is separable, with two conserved quantities that look like "effective energies,"

...
\[ e_u = \frac{1}{2} p_u^2 + \frac{1}{2} u^4 - \epsilon u^2 , \quad (16a) \]

\[ e_v = \frac{1}{2} p_v^2 - \frac{1}{2} v^4 - \epsilon v^2 . \quad (16b) \]

Particles start from the origin \( u = 0, v = 0 \) at fixed "total energy" \( e_u + e_v = 2 \) moving in any direction. The motion in \( u \) is oscillatory, and there are two unstable POs that sit on top of barriers at \( v = \pm \sqrt{-\epsilon} = v_b \) with \( e_v = \epsilon^2/2 \equiv e_b \).

Fig. 3. Potential-energy contours for the Stark Hamiltonian.

We will show that the closed orbits form patterns analogous to those found for the harmonic barrier. They form orderly sequences approaching the unstable POs, and formulas similar to Eqs. (10) and (14) can be derived. There is only one difference. Below the barriers, the \( v \)-motion is bounded and oscillatory, whereas the \( y \) motion of the harmonic barrier was unbounded. Therefore, in the present case, closed orbits form sequences labeled by two integers. This was evident in Fig. 1.

First we expand Eq.(16b) around either barrier point:

\[ e_v = e_b + \frac{1}{2} p_v^2 + \epsilon (v-v_b)^2 + \ldots . \quad (17) \]

Comparing this with our discussion below Eq.(2), we see that for \( \epsilon < 0 \), the neighbors of the unstable PO diverge from it as \( \exp(2 \sqrt{-\epsilon} t) \), and we define the Liapunov factor as
\[ \lambda_{\alpha n} = \omega_{\alpha n} T_{\alpha n} = 2\sqrt{-\varepsilon} T_{\alpha n}. \]  

The period of the unstable orbit, and \( \omega_{\alpha n} \) is the force constant producing the divergence.

The general orbit is quasiperiodic. Periodic orbits occur whenever the periods of \( u \) and \( v \) motions are commensurate, \( T_u/T_v = m/l \). Moreover, because of the symmetry of the system, every orbit that is closed at the origin is periodic. It is convenient to label the closed orbits by the un reduced fraction \( m/l \).

If the fraction is in lowest terms, then there are \( m \) half-cycles of \( v \) motion and \( l \) half-cycles of \( u \) motion before the first closure; otherwise, the unreduced fraction represents a subsequent closure of such an orbit.

We consider sequences with \( m \) fixed and \( l \) increasing. For example, we consider the sequence \( 3/5, 3/6, 3/7, 3/8, 3/9 \ldots \), with the \( 3/6 \) and \( 3/9 \) being respectively the second and the third closures of the \( 1/2 \) and \( 1/3 \) orbits. For \( m=1 \), each orbit approaches one of the barriers, and then returns to the origin. This sequence looks just like the sequence found for the harmonic barrier. If \( m=2 \), the orbits approach both barriers once before returning to the origin. If \( m=3 \), they have \( 1\frac{1}{2} \) cycles of \( v \)-motion before closure, and so on.

### 2.1. Classical Actions and Amplitudes

The classical action of each closed orbit is the sum of the \( u \)-action and \( v \)-action, and each of those can be regarded as a function of \( \varepsilon \) and \( \varepsilon_v \)

\[ S_{mf}(\varepsilon, \varepsilon_v) = lS_u(\varepsilon, \varepsilon_v) + mS_v(\varepsilon, \varepsilon_v). \]  

\[ S_v(\varepsilon, \varepsilon_v) = \oint (2\varepsilon_v + v^4 + 2\varepsilon v^2)^{1/2} dv \]  

\[ S_u(\varepsilon, \varepsilon_v) = \oint (4 - 2\varepsilon_v - u^4 + 2\varepsilon u^2)^{1/2} du. \]

The limiting value of \( S_u(\varepsilon, \varepsilon_v) \) is half the action of the unstable PO, \( S_{u*} \). In a sequence, when \( l \) is large, \( \varepsilon_v \) approaches the limiting value \( \varepsilon^{7/2} \), so \( S_u \) and \( S_v \) approach limits. Hence the action difference of two successive COs is related to the action of the unstable orbit:
\[
\lim_{l \to \infty} \left( S_m \frac{T_m}{T} - S_m \right) = S_u (\epsilon, \epsilon^2/2) = S_u \frac{1}{2} .
\] (22)

We can also show that for large \( l \), the classical amplitudes of successive closed orbits in a sequence vary as
\[
A_m \frac{T_m}{T} = \exp \left( -\frac{\omega_m}{4m} \right) \\
= \exp \left( -\frac{\omega_u T_u}{4m} \right) \\
= \exp \left( -\sqrt{|\epsilon|} \frac{T_u}{2m} \right) .
\] (23)

The proof takes a few pages; it is given in Ref. 7.

3. Conclusion

The harmonic barrier model is simple, exactly solvable, and gives a clear picture of the patterns of closed orbits that have been found to occur in many systems.

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References


